# Step 1 Generate or Compile Data Opening the first of the state of th

## Step 2

#### Select Thermodynamic Model

$$\begin{split} P &= \frac{RT}{V - b} - \frac{a}{V^2 - ubV + wb^2} \\ a_m &= \sum_i \sum_j y_i y_j \sqrt{a_i a_j} (1 - \kappa_{ij}) \\ a_j &= 0.421875 \frac{R^2 T_{Cj}^2}{P_{Cj}} \alpha_j \\ b_j &= 0.125 \frac{RT_{Cj}}{P_{Cj}} \\ b_m \sum_{i=1}^N x_i &= 1 \end{split}$$

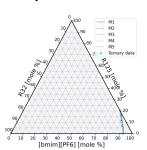


### Step 3

**Estimate Parameters** 

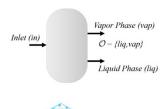


## Step 4 Calculate Phase Equilibrium



### Step 5

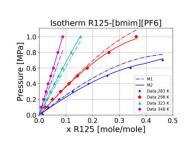
Perform Process
Calculations



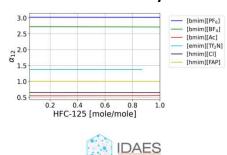


## Step 6

Assess Quality of Fit

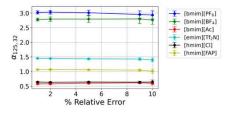


# Step 7 Screen ILs via Relative Volatility



## <u>Step 8</u>

Quantify Uncertainty & Inform Experiments





PYOMO